

Supplementary Material for

Metabolomics Analysis of Different Quinoa Cultivars Based on UPLC-ZenoTOF-MS/MS and Investigation into Their Antioxidant Characteristics

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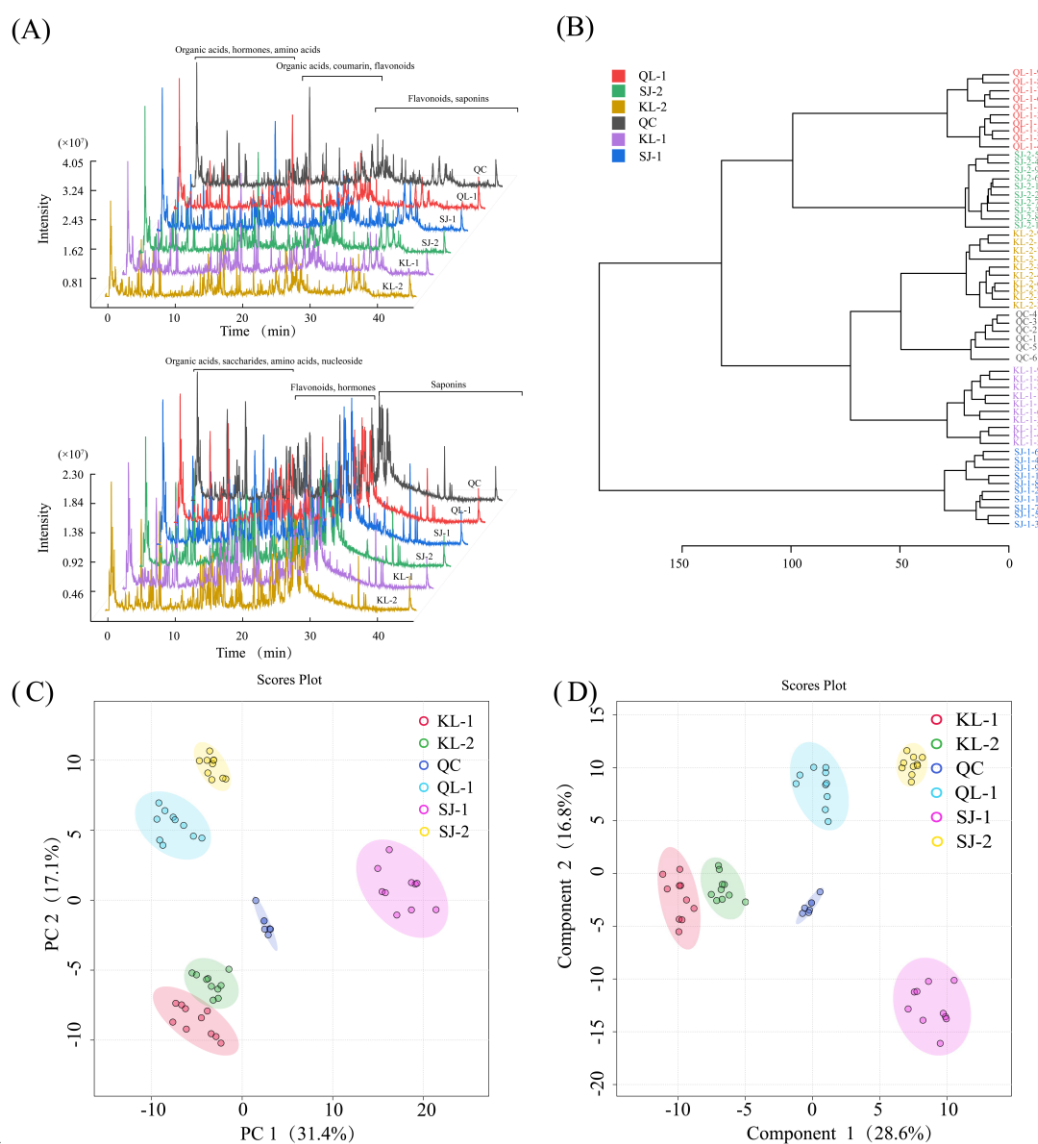


Figure S1. Isolation and identification of metabolites in different cultivars of quinoa. Total ion chromatogram of metabolite molecular species from different cultivars of quinoa under positive (Upper one) and negative (Lower one) ion mode (A). Hierarchical cluster dendritic diagram from different cultivars of quinoa under positive and negative ion mode (B). PCA score plot (C) and PLS-DA score plot (D) of identified metabolites in different cultivars of quinoa.

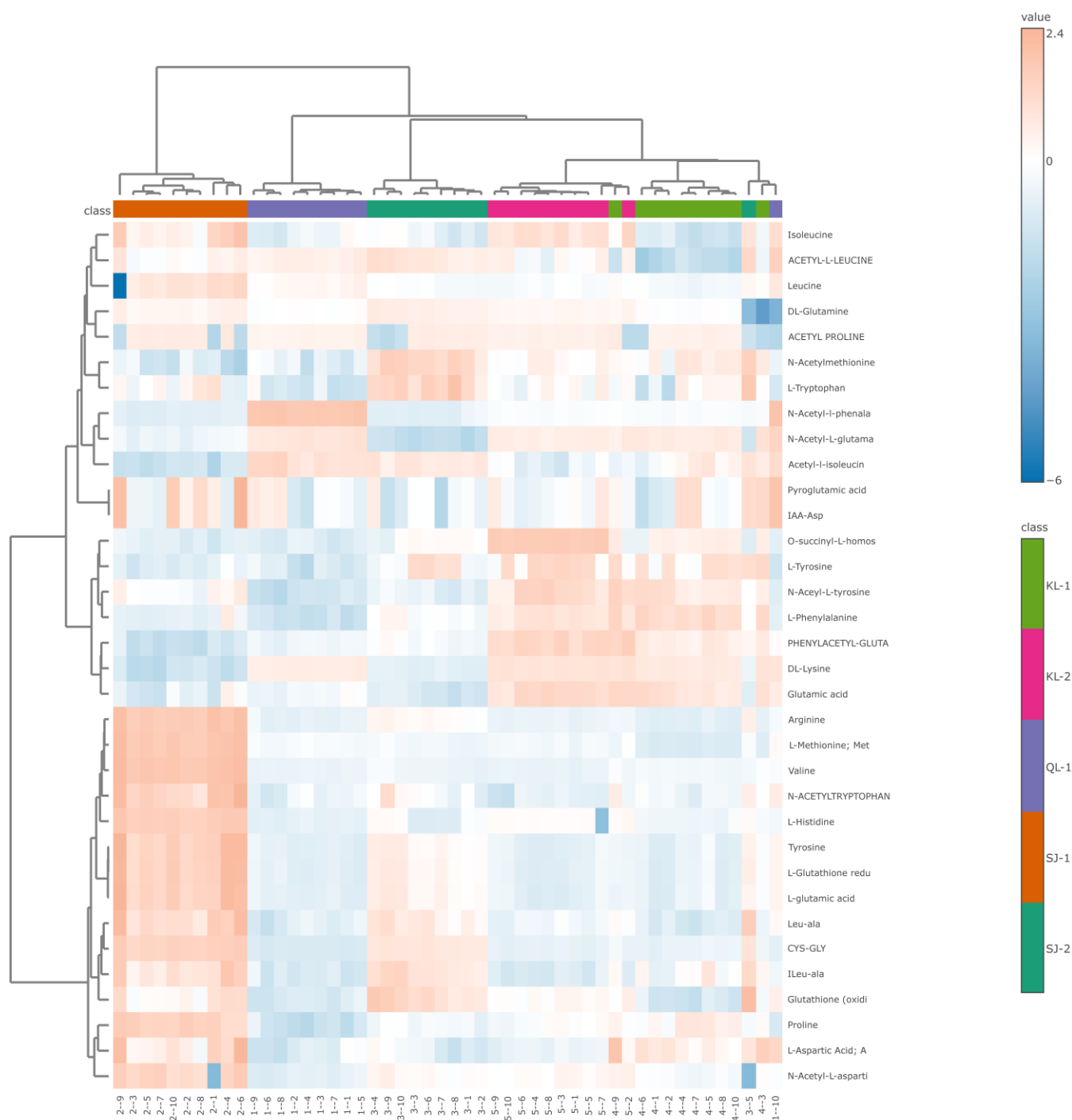


Fig S2 Heatmaps based on top 25 amino acids/peptides in different varieties of quinoa. Colors represent different concentrations indicated by the color bar.

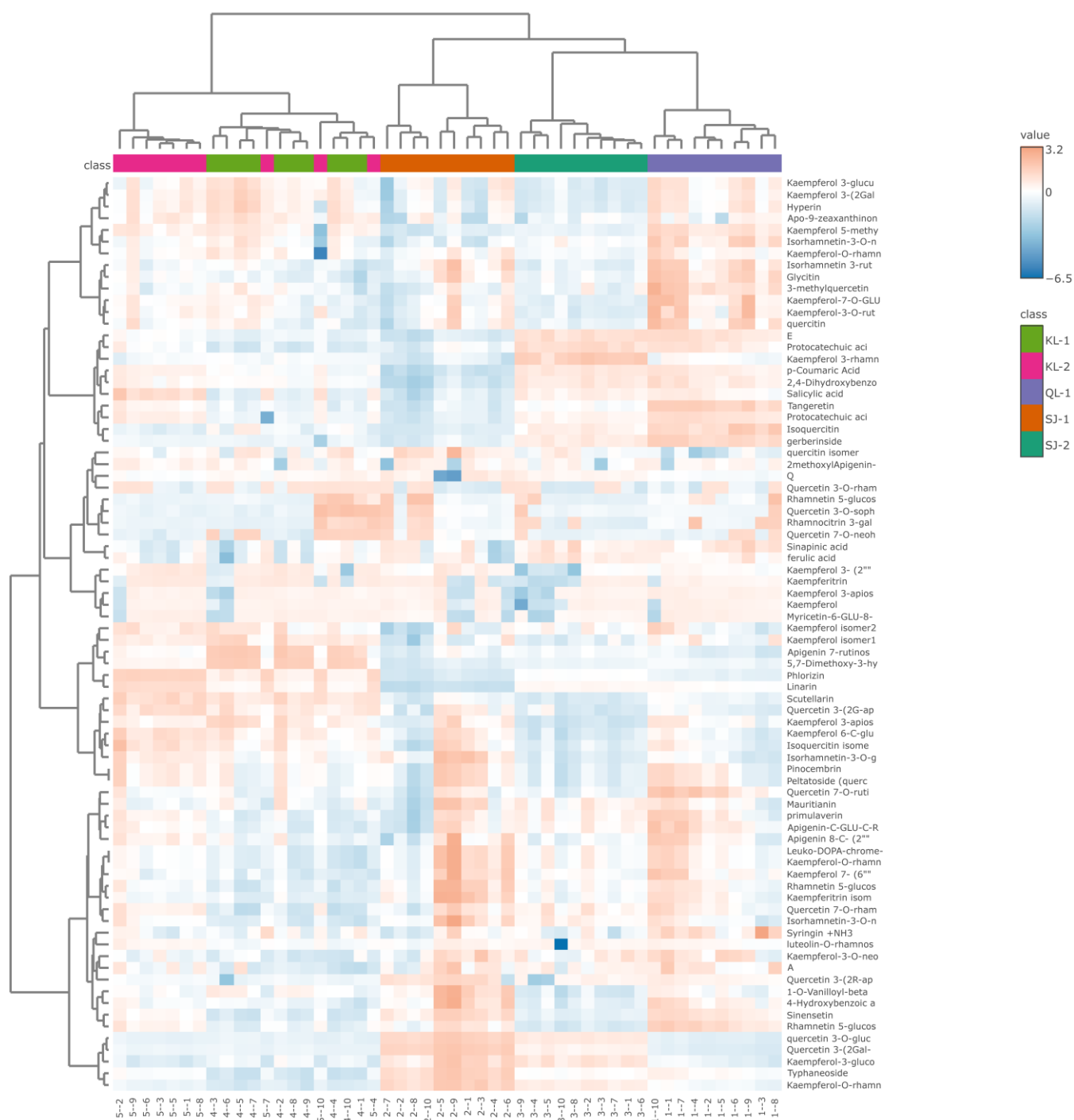


Fig S3 Heatmaps based on top 25 phenolic acids in different varieties of quinoa. Colors represent different concentrations indicated by the color bar.

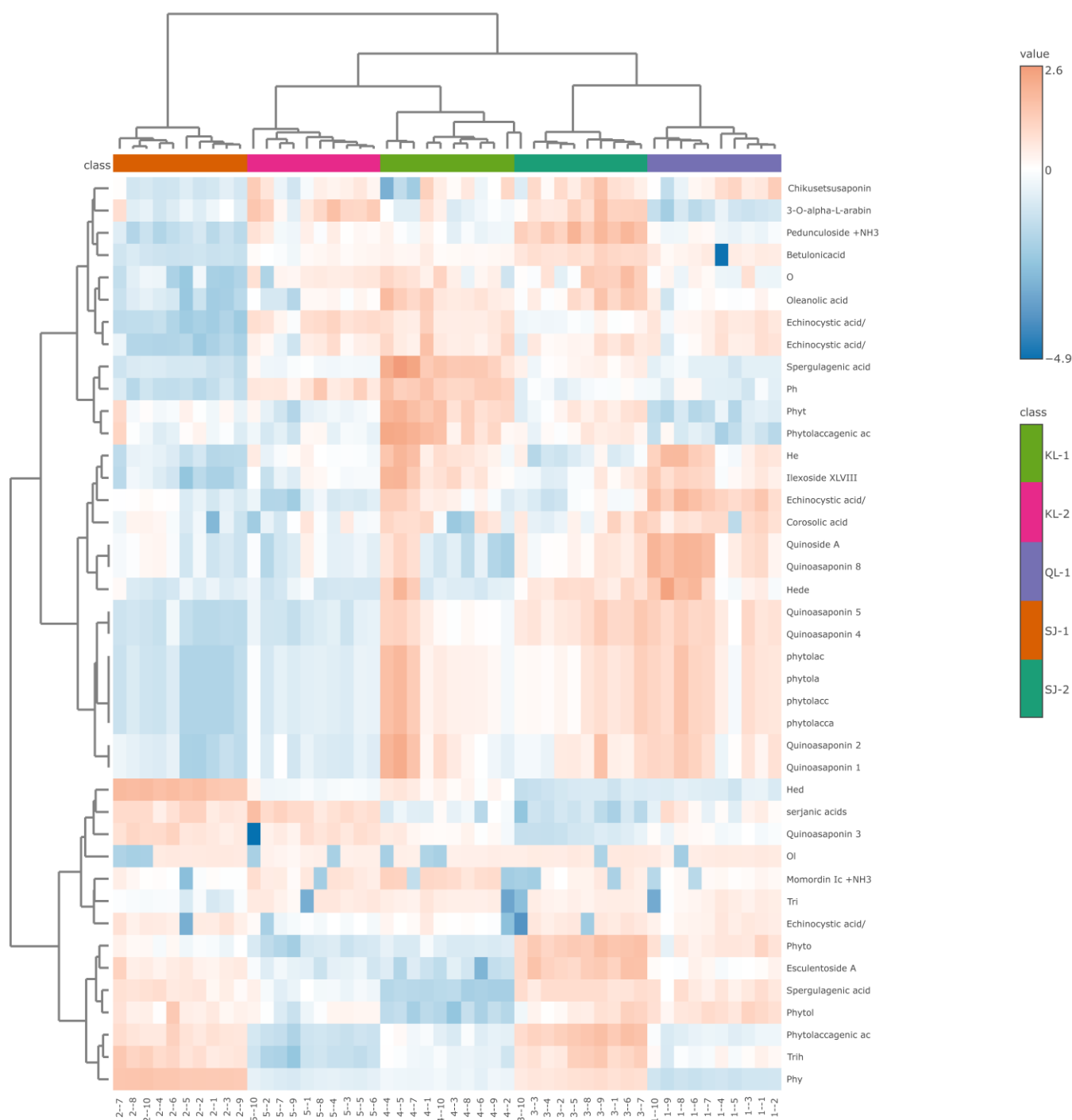


Fig S4 Heatmaps based on top 25 saponins in different varieties of quinoa. Colors represent different concentrations indicated by the color bar.

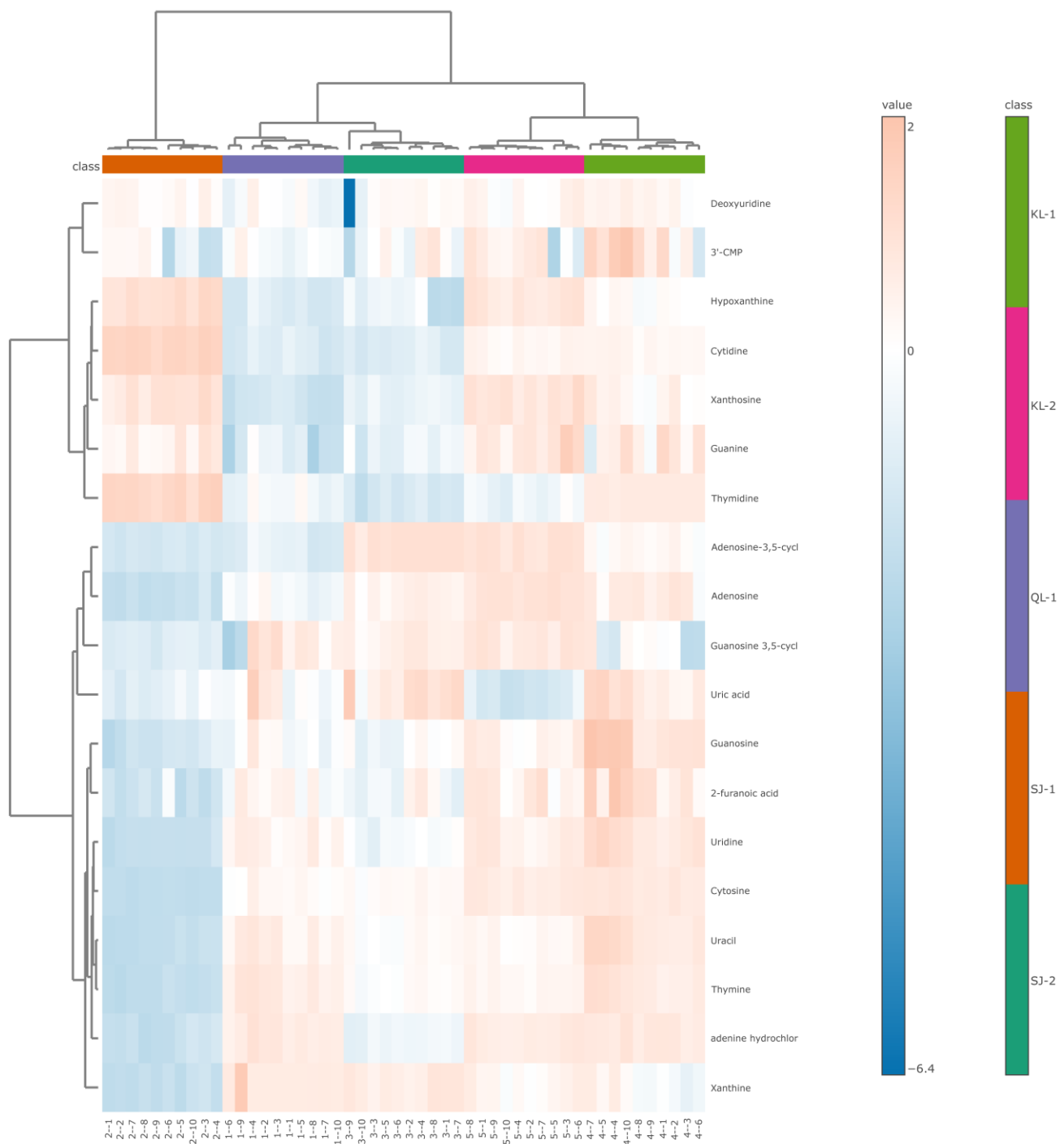


Fig S5 Heatmaps based on top 25 nucleosides in different varieties of quinoa. Colors represent different concentrations indicated by the color bar.

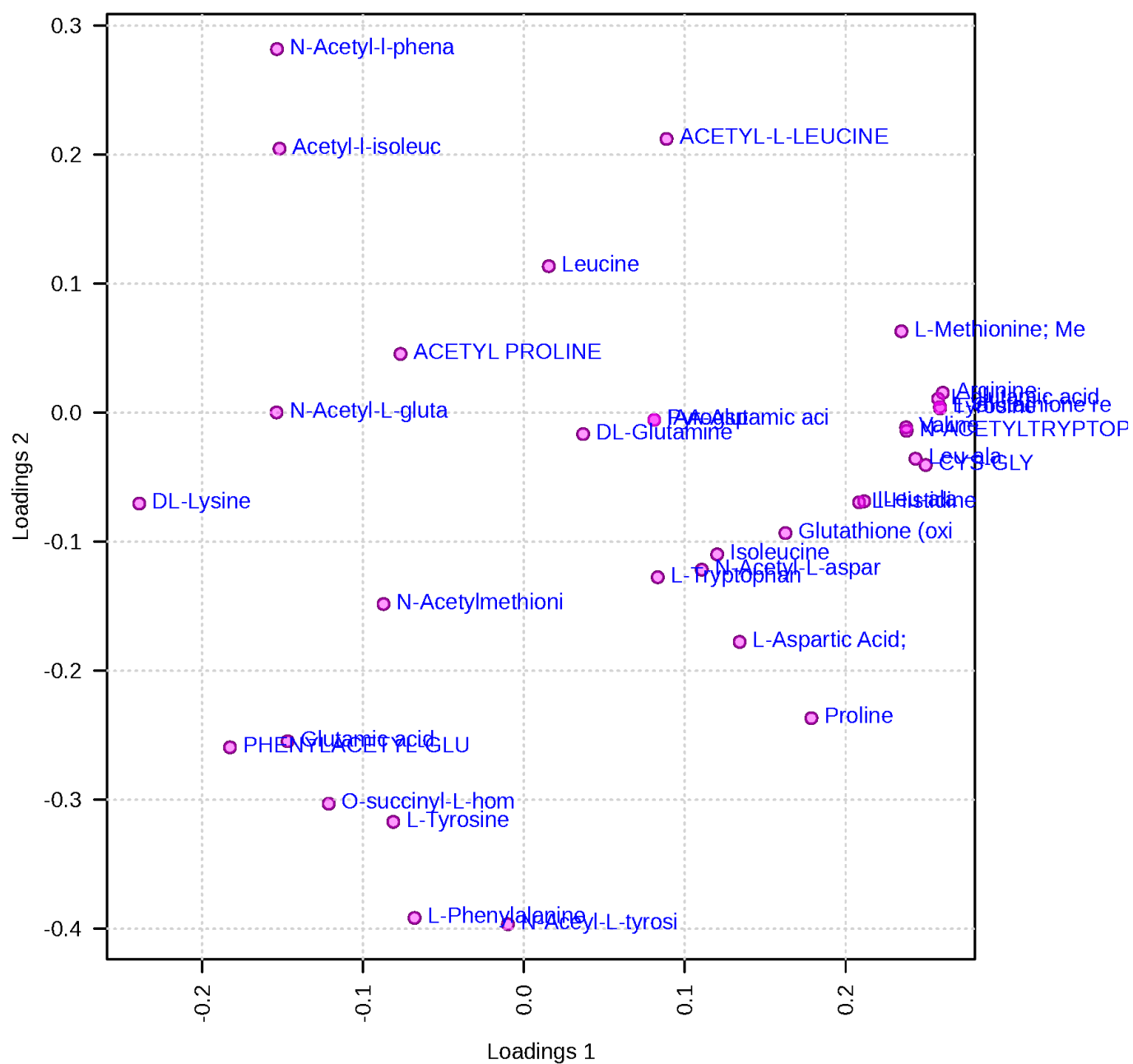


Fig S6 Loading plots of amino acids/peptides in different varieties of quinoa.

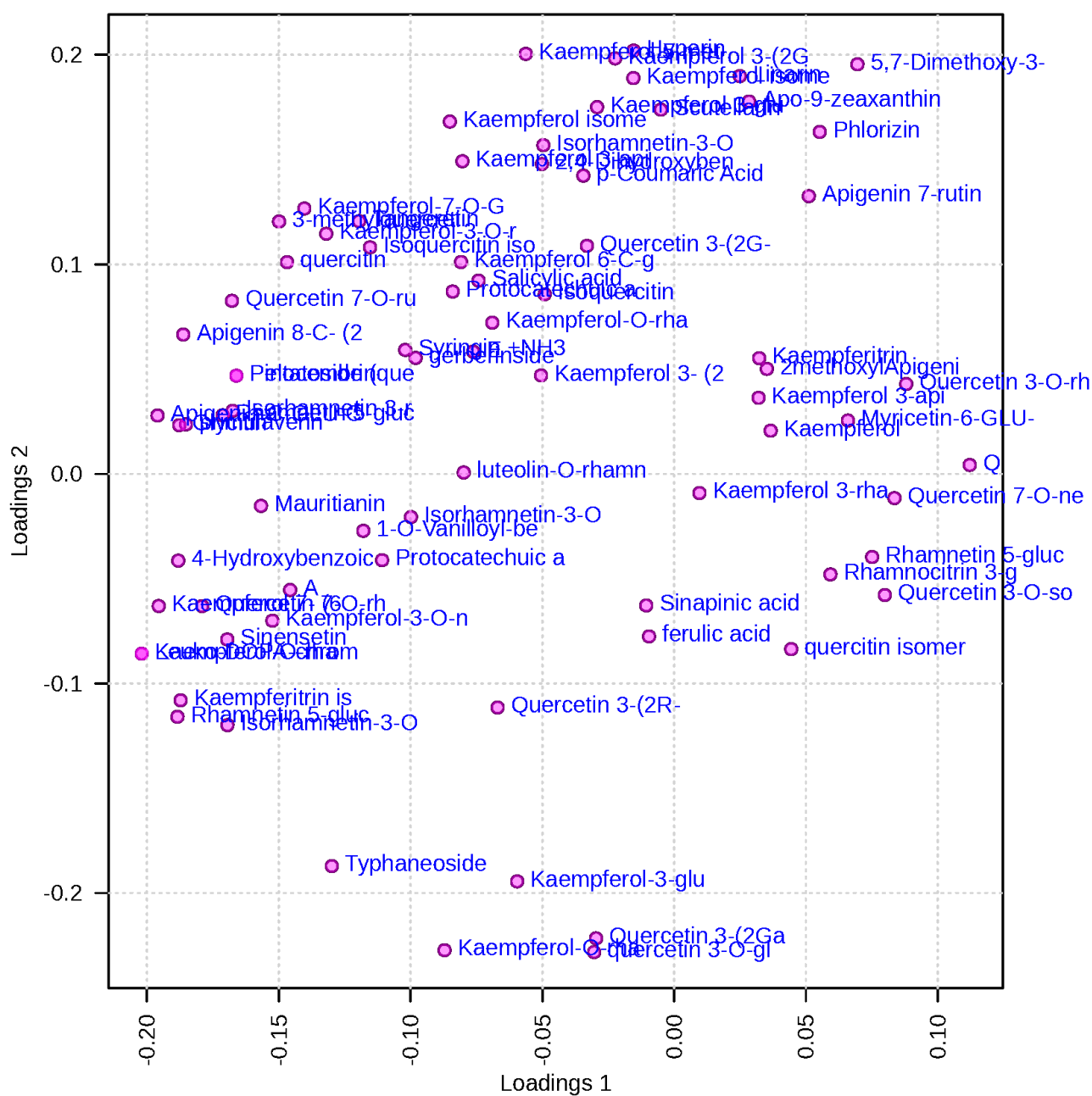


Fig S7 Loading plots of phenolic acids in different varieties of quinoa.

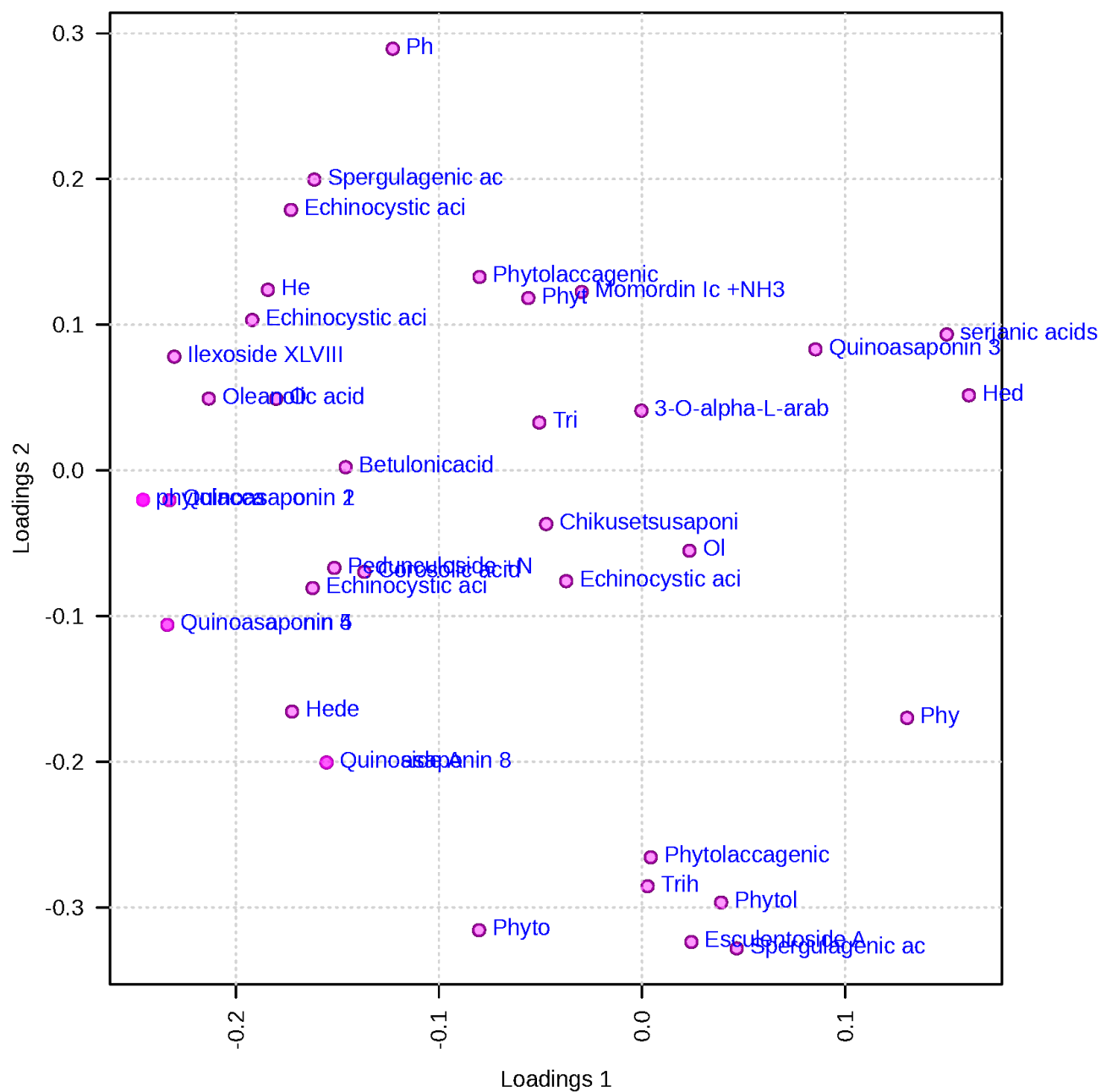


Fig S8 Loading plots of saponins in different varieties of quinoa.

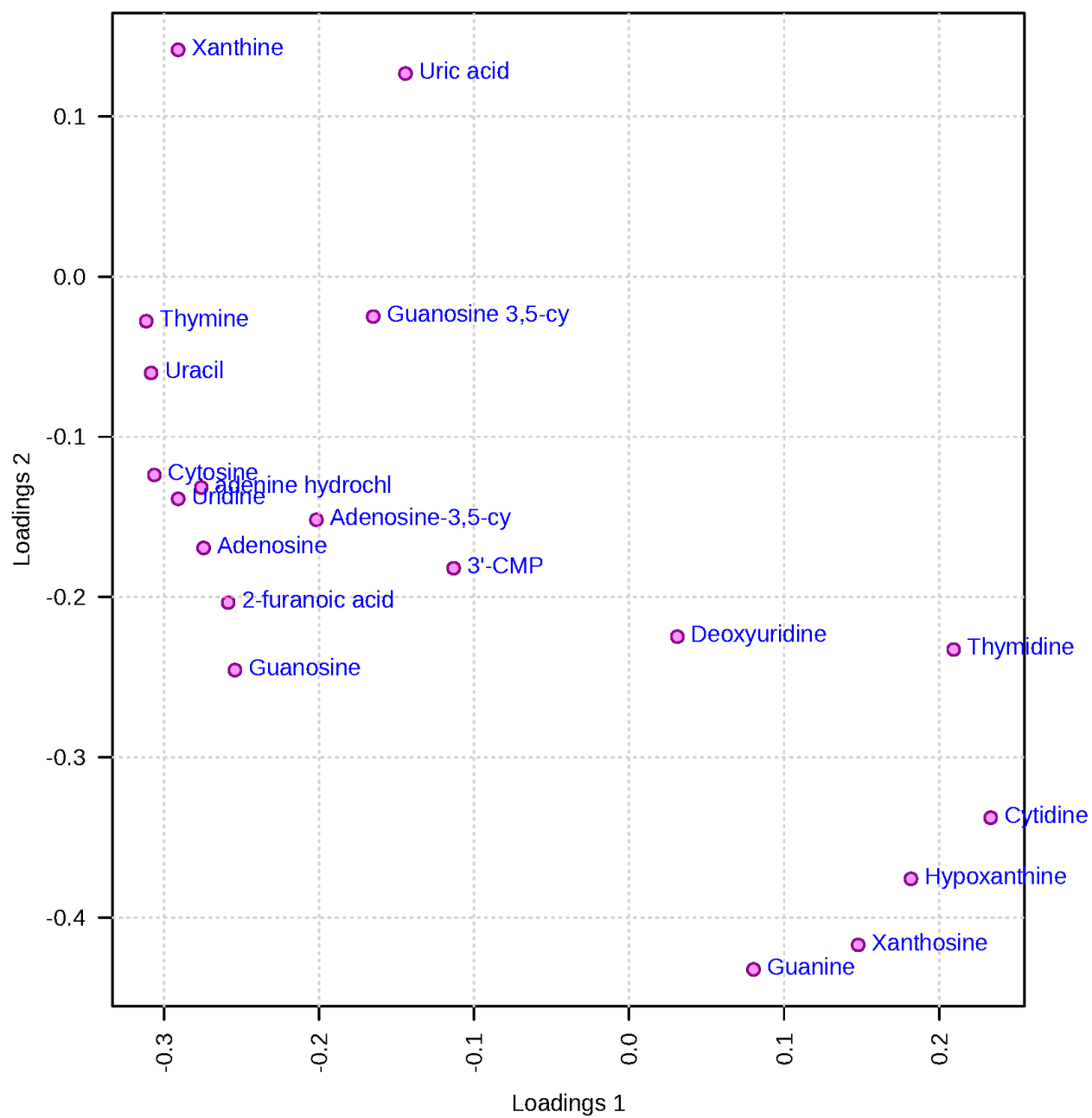



Fig S9 Loading plots of amino nucleosides in different varieties of quinoa.

Tab S1 Types of metabolites detected in different varieties of quinoa.

Metabolite type	Metabolites
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Amino acid/peptide	ACETYL PROLINE Acetyl-l-isoleucine ACETYL-L-LEUCINE CYS-GLY DL-Glutamine DL-Lysine Glutamic acid Glutathione (oxidized) IAA-Asp lLeu-ala Isoleucine L-Aspartic Acid; Asp Leu-ala Leucine L-Glutathione reduced L-Histidine L-Methionine; Met H -H L-Phenylalanine L-Tryptophan L-Tyrosine N-Acetyl-L-aspartic acid N-Acetyl-L-glutamate N-Acetyl-l-phenalanine N-Acetylmethionine N-ACETYLTRYPTOPHAN N-Aceyl-L-tyrosine O-succinyl-L-homoserine PHENYLACETYL-GLUTAMINE Proline Pyroglutamic acid Tyrosine Valine Arginine

	L-glutamic acid
Sesquiterpene	Curdione Patchouli alcohol (loss H ₂ O)
Nucleoside	2-furanoic acid 3'-CMP adenine hydrochloride Adenosine Adenosine-3,5-cyclic phosphate cAMP Cytidine Cytosine Deoxyuridine Guanine Guanosine Guanosine 3,5-cyclic monophosphate Hypoxanthine Thymidine Thymine Uracil Uric acid Uridine Xanthine Xanthosine
Phenolics	2,4-Dihydroxybenzoic acid 4-Hydroxybenzoic acid ferulic acid p-Coumaric Acid Protocatechuic acid Protocatechuic acid-3-glucoside Salicylic acid Sinapinic acid 1-O-Vanilloyl-beta-D-glucose E 2methoxylApigenin-O-GLU-O-Rha 3-methylquercetin A 5,7-Dimethoxy-3-hydroxyflavone Apigenin 7-rutinoside Apigenin 8-C- (2",3"-diacetylglucoside) Apigenin-C-GLU-C-Rha Apo-9-zeaxanthinone gerberinside Glycitin

	Hyperin
	Isoquercitin
	Isoquercitin isomer
	Isorhamnetin 3-rutinoside
	(Narcissoside)
	Isorhamnetin-3-O-glucoside
	Isorhamnetin-3-O-neohespeidoside
	Isorhamnetin-3-O-neohespeidoside isomer
	Kaempferitrin
	Kaempferitrin isomer
	Kaempferol
	Kaempferol 3- (2"- (E) -p-coumaroyl- alpha-L-arabinofuranoside) -8-C- rhamnoside
	Kaempferol 3-(2Gal- apiosylrobinobioside)
	Kaempferol 3-apiosyl-(1->2)- galactoside
	Kaempferol 3-apiosyl-(1->4)- rhamnoside-7-rhamnoside
	Kaempferol 3-glucuronide
	Kaempferol 3-rhamnoside-7-xyloside
	Kaempferol 5-methyl ether
	Kaempferol 6-C-glucoside-8-C- rhamnoside
	Kaempferol 7- (6"-p-succinylglucoside)
	Kaempferol isomer1
	Kaempferol isomer2
	Kaempferol-3-glucoside (Astragalin)
	Kaempferol-3-O-neohespeidoside
	Kaempferol-3-O-rutinoside
	Kaempferol-7-O-GLU
	Kaempferol-O-rhamnoside isomer1
	Kaempferol-O-rhamnoside isomer2
	Kaempferol-O-rhamnoside isomer3
	Leuko-DOPA-chrome-glucoside
	Linarin
	luteolin-O-rhamnoside-GLU
	Mauritianin
	Myricetin-6-GLU-8-Xyl

	<p>Peltatoside (quercetin-3-arabinoglucoside)</p> <p>Phlorizin</p> <p>Pinocembrin</p> <p>primulaverin</p> <p>Quercetin 3-(2Gal-rhamnosyl-robinobioside)</p> <p>Quercetin 3-(2G-apiosylrutinoside)</p> <p>Quercetin 3-(2R-apiosylrutinoside)</p> <p>quercetin 3-O-glucuronide</p> <p>Quercetin 3-O-rhamnosyl-(1->6)-galactoside</p> <p>Quercetin 3-O-sophoroside</p> <p>Quercetin 7-O-neohespeidoside</p> <p>Quercetin 7-O-rhamnosyl-(1->6)-galactoside</p> <p>Quercetin 7-O-rutinoside</p> <p>Q</p> <p>quercitin</p> <p>quercitin isomer</p> <p>Rhamnetin 5-glucoside</p> <p>Rhamnetin 5-glucoside isomer1</p> <p>Rhamnetin 5-glucoside isomer2</p> <p>Rhamnocitrin 3-galactoside</p> <p>Scutellarin</p> <p>Sinensetin</p> <p>Syringin +NH3</p> <p>Tangeretin</p> <p>Typhaneoside</p>
hormone	<p>Corticosterone</p> <p>ecdysterone</p> <p>Indole</p> <p>Norethisterone acetate</p>
pigment	<p>4,5-seco-DOPA</p> <p>Amaranthin</p> <p>Betanin</p> <p>DOPA-betaxanthin</p>
alkaloid	<p>N-trans-Feruloyl tyramine</p> <p>Sinapine</p> <p>Trigonelline</p>
sugar	<p>D-Glucose</p> <p>D-Sucrose</p>

	nystose RAFFINOSE Sibiricose A1 Sibiricose A5 Stachyose D-Glucose 1-phosphate Fungitetraose Po Pom
vitamin	4-Pyridoxic Acid Nicotinic acid Vitamin B2 Vitamin B4 Vitamin B5
coumarin	6-Methylcoumarin Cinnamaldehyde Coumarin Scoparone 2-Aminoadipic acid 2-ISOPROPYLMALIC ACID 3-(4-Hydroxyphenyl)lactate anthranilic acid CITRIC ACID DL-3-Aminoisobutyric acid DL-Malic acid -H glutaconic acid hexadecylitaconic acid Hexaric acid L-Threonic acid methylene succinic acid Pantothenic Acid Pipecolic acid Pipicolinic acid Succinic acid trans-3-indole-acrylic acid Vanillic acid Glycyrrhetic acid
organic acid	
saponin	3-O-alpha-L-arabinopyranosylserjanic acid 28-O-beta-D-glucopyranosyl ester 3β,23,30 trihydroxy olean-12-en-28-oic acid

3 β ,23,30 trihydroxy olean-12-en-28-oic
acid isomer
Betulonicacid
Chikusetsusaponin IVa
Corosolic acid
Echinocystic
acid/Hederagenin/Queretaroic acid 1
Echinocystic
acid/Hederagenin/Queretaroic acid 2
Echinocystic
acid/Hederagenin/Queretaroic acid 3
Echinocystic
acid/Hederagenin/Queretaroic acid 4
Esculentoside A
Ilexoside XLVIII
Momordin Ic +NH₃
Oleanolic acid
oleanolic acid 3-O-[α -L-
arabinopyranosyl-(1-3)- β -D-
glucopyranosyl]-28-O- β -D-
glucopyranoside
oleanolic acid 3-O- β -D-glucopyranosyl-
28-O- β -D-glucopyranoside
Pedunculoside +NH₃
Phytolaccagenic acid
phytolaccagenic acid 3-O- [α -L-
arabinopyranosyl-(1-3)- β -D-
glucuronopyranosyl]- 28-O- β -D-
glucopyranoside
phytolaccagenic acid 3-O- [α -L-
arabinopyranosyl-(1-3)- β -D-
glucuronopyranosyl]- 28-O- β -D-
glucopyranoside isomer
phytolaccagenic acid 3-O-[β -D-
glucopyranosyl-(1-4)- β -D-
glucopyranosyl-(1-4)- β -D-
glucopyranosyl]-28-O- β -D-
glucopyranoside
phytolaccagenic acid 3-O-[β -D-
glucopyranosyl-(1-4)- β -D-
glucopyranosyl]-28-O- β -D-
glucopyranoside

phytolaccagenic acid 3-O-[β -D-glucopyranosyl-(1-4)- β -D-glucopyranosyl]-28-O- β -D-glucopyranoside isomer

Phytolaccagenic acid isomer

phytolaccagenic acid-3-O- β -D-glucopyranosyl-28-O- β -D-glucopyranoside

phytolaccagenic acid-3-O- β -D-glucopyranosyl-28-O- β -D-glucopyranoside isomer1

phytolaccagenic acid-3-O- β -D-glucopyranosyl-28-O- β -D-glucopyranoside isomer2

phytolaccagenic acid-3-O- β -D-glucopyranosyl-28-O- β -D-glucopyranoside isomer3

Quinoasaponin 1

Quinoasaponin 2

Quinoasaponin 3

Quinoasaponin 4

Quinoasaponin 5

Quinoasaponin 8

Quinoside A

serjanic acids

spergulagenic acid 3-O-[α -L-arabinopyranosyl-(1-3)- β -D-glucuronopyranosyl]-28-O- β -D-glucopyranoside

hedeagenin 3-O-[α -L-arabinopyranosyl-(1-3)- β -D-glucuronopyranosyl]-28-O- β -D-glucopyranoside

hedeagenin 3-O-[α -L-arabinopyranosyl-(1-3)- β -D-glucuronopyranosyl]-28-O- β -D-glucopyranoside isomer1

hedeagenin 3-O-[α -L-arabinopyranosyl-(1-3)- β -D-glucuronopyranosyl]-28-O- β -D-glucopyranoside isomer2

	spergulagenic acid 3-O-[β -D-glucopyranosyl-(1-2)- β -D-glucopyranosyl-(1-3)- α -L-arabinopyranosyl]-28-O- β -D-glucopyranoside
other	(Z)-3-[4-methoxy-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoic acid 13-Docosenamide 13-Oxo-9,11-tridecadienoic acid 1-amino-naphthalene 1-O-Vanilloyl-beta-D-Galactose 2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one 3-hydroxytyramine hydrochloride 4-hydroxy-6-methyl-2-pyron 7-hydroxy-4-methyl-chromen-2-one 9-(2,3-dihydroxypropoxy)-9-oxononanoic acid Acetophenone C18:2-glycer-Glu Choline ethyl 6-(4-hydroxyphenyl)-4-methyl-2-oxo-1,3,6-trihydropyrimidine-5-carboxylat e Gingerglycolipid B Levodopa Methyl linoleate N-trans-Isoferuloyl-3-O-methyldopamine Phosphocholine pinellic acid piperidine Momordin IIc Sambucinol H -H Methoxsalen

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